# EFFECTS OF DIPE PRODUCTION ECONOMICS ON THE REFINING VALUE OF ETHANOL

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# GASOLINE BLENDSTOCK AND ETHERIFICATION FEEDSTOCK

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## Effects of DIPE Production Economics on the Refining Value of Ethanol as Gasoline Blendstock and Etherification Feedstock

### Background

This report describes an analysis of the effects on ethanol's long-term refining value of changes in the economics of producing di-isopropyl ether (DIPE), an oxygenated gasoline blendstock likely to compete with ethanol and MTBE in the future. The work described in this report was carried out as part of Task 1 of NREL Subcontract No. ACG-5-15356-01 (21 September 1995).

This work is a sensitivity analysis extending prior work performed for NREL to analyze ethanol's value in the U.S. petroleum refining sector. The prior work was performed under Subcontract No. AAW-4-14125-01 and documented in that subcontract's Report 5, *The Refining Value of Ethanol as Gasoline Blendstock and Etherification Feedstock* (18 July 1995) [MP95].

This report should be considered a supplement to the 18 July report. In general, the work described here embodies the same methodology, data, and assumptions as did the prior work. The reader interested in these matters should refer to the 18 July report.

The prior work (1) explored the technical and economic determinants of ethanol's refining value as a gasoline blendstock and as an etherification feedstock and (2) developed aggregate demand functions for fuel-grade ethanol in the U.S. refining sector, for the year 2010.[1] The estimated demand functions correspond to various crude oil and natural gas prices projected for 2010 in DoE's *1995 Annual Energy Outlook* and reflect assumptions regarding future refining technology, refining economics, and public policies bearing on gasoline quality and composition.

The sensitivity analysis described in this report explores the implications of one set of assumptions in the prior work -- that bearing on the economics of DIPE production in U.S. refineries in 2010. The prior work reflected the latest published quotation (by UOP Inc., the primary licensor of the DIPE process) of investment requirements and operating costs for DIPE production in a refinery-scale unit. The analysis described in this report explores the effects on ethanol's refining value of possible changes in two key determinants of the overall economics of refinery-based DIPE production:

- The investment requirements for refinery-based DIPE production, and
- The level of demand for refinery propylene -- the feedstock for producing DIPE -- in the petrochemical sector.

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[1] We use the term "demand function" to refer to the relationship between the refining value of ethanol and the volume of ethanol used by refineries, either as an ether feedstock or as a direct gasoline blendstock. Refer to the previous report for a discussion of the distinction between the market value and the refining value of ethanol.

(Demand in the petrochemical sector pulls propylene out of the refining sector and thereby can affect the value of propylene in the refining sector -- and hence the economics of DIPE use.)

The third key determinant of DIPE economics is the price of crude oil. This sensitivity study does not cover the crude oil price level because the effects of crude oil price on ethanol's refining value were delineated in the prior work.

The discussion that follows is in five sections:

1. Summary of Results
2. Techno-Economics of DIPE Production and Use
3. Likely Evolution of DIPE Investment Costs Over Time
4. Methodology for The Analysis
5. Results of The Analysis

## Summary of Results

The results of this analysis indicate that investment in significant volumes of DIPE capacity would reduce ethanol's refining value -- but only at high volumes of ethanol use (that is, above 500 M Bbl/day). For ethanol volumes below 500 M Bbl/day, ethanol's refining value may be viewed (for all practical purposes) as independent of DIPE capacity. However, increasing levels of DIPE capacity, in excess of 150 M Bbl/day, would progressively reduce the threshhold volume of ethanol use -- the volume above which ethanol's refining value would decrease sharply with further increases in volume.

Such levels of DIPE capacity appear likely should RFG constitute 50% of the U.S. gasoline pool. DIPE capacity is attractive in certain refinery settings now, with the current investment cost per unit of DIPE capacity. The investment cost for DIPE capacity is likely to be lower in 2010 than today; that is, lower than the value used in our prior analysis. The economic incentive for DIPE capacity is essentially independent of the level of demand for refinery propylene in the petrochemical sector.

## Techno-Economics of DIPE Production and Use

### *Introduction*

DIPE is an oxygenated gasoline blendstock with attractive blending properties, comparable to those of ETBE.

During the '50s, the predecessor to today's Mobil Corporation identified DIPE as a high-octane gasoline blendstock and delineated the chemistry of DIPE synthesis. However, DIPE did not enter commercial use because its indicated cost of production was greater than its octane value.

The oxygenated and RFG programs established by the Clean Air Act Amendments of 1990 (CAAA) created an additional standard of value -- oxygen value -- for gasoline blendstocks. The CAAA thereby rekindled interest in DIPE and stimulated efforts to develop a commercial process for DIPE production. In the first quarter of 1994, UOP Inc. (a leading licensor of refining process technology) announced a new process for refinery production of DIPE with attractive economics [UOP94]. The process is commercial and available under license.

The new DIPE process arrived too late for the refining industry's additions to capital stock to comply with the federal Phase 1 and the California RFG programs. But our prior work indicated that DIPE is likely to play a key role when the refining industry is next called upon to expand its capacity to produce reformulated gasolines or to meet more stringent emission standards (such as the federal Phase 2 RFG standards, to take effect in 2000).

*Basic DIPE Chemistry*

Large-scale DIPE production in a refinery involves combining refinery propylene with water in a sequence of chemical reactions that can be summarized as:

$$2C_3H_6 \quad + \quad H_2O \quad \text{-------->} \quad C_3H_7OC_3H_7$$

(Propylene) (DIPE)

The source of DIPE's oxygen is ordinary water -- not an alcohol (i.e., ethanol or methanol). The sole hydrocarbon feed to a DIPE plant is refinery propylene.

*Propylene Dispositions*

Refinery propylene is produced as a by-product in various refinery process units -- most importantly the fluid catalytic cracking (FCC) unit. Refinery propylene has four dispositions in current U.S. refining operations [UOP94]:

- Sales to the petrochemical industry (48%)
- Feedstock for refinery production of *propylene alkylate* (36%)
- Feedstock for refinery production of *polymer gasoline* (13%)
- Refinery fuel and LPG ( 3%)

These percentages apply to the total U.S. refining sector.

*Propylene alkylate* and *polymer gasoline* are conventional, high-octane gasoline blendstocks. Propylene alkylate is produced by combining propylene with iso-butane, another FCC by-product stream. Polymer gasoline is produced from propylene alone.

Propylene alkylate is produced in process units that also produce (or can produce) butene ($C_4$) alkylate and amylene ($C_5$) alkylate, from (respectively) mixed butene and mixed amylene streams. These streams too are FCC by-products.

In general, refineries do not produce propylene "on purpose"; it is a normal by-product of FCC operations. However, a refinery can produce significant additional volumes of "on purpose" propylene through suitable adjustment of FCC operating conditions and use of special FCC catalysts tailored to maximize production of light olefins, including propylene. This flexibility with regard to propylene production has a strong bearing on the results of this study.

*Blendstock Properties*

**Table 1** summarizes key gasoline blending properties for DIPE, the oxygenated blendstocks now in commercial use, alkylate, and polymer gasoline.

The properties of alkylate and polymer gasoline are of interest in this context because production of DIPE could draw propylene away from production of alkylate and/or polymer gasoline.

**Table 1: Blending Properties of Oxygenated and Propylene-Derived Blendstocks**

| Blendstock | Blending Octane (R + M)/2 | Blending Rvp (psi) | Oxygen Content (Wt. %) | Olefin Content (Wt.%) |
|---|---|---|---|---|
| Ethanol | 115 | Raises blend Rvp by 1 psi | 34.7 | 0 |
| <u>Ethers</u> | | | | |
| MTBE | 110 | 8-9 | 18.2 | 0 |
| ETBE | 111 | 3-5 | 15.7 | 0 |
| TAME | 105 | 3-4 | 15.7 | 0 |
| DIPE | 105 | 4-5 | 15.7 | 0 |
| <u>Propylene-Derived</u> | | | | |
| Propylene alkylate | 89.5 | 4 | 0 | 0 |
| Polymer gasoline | 87.5 | 2 | 0 | 100 |

*Consequences of DIPE Production*

As the preceding discussion suggests, introducing DIPE into the gasoline pool offers several benefits to refiners.

- DIPE production would insulate refiners from the vagaries of ethanol, methanol, MTBE, and other external markets and from fluctuations in merchant oxygenate prices.

DIPE can be produced entirely within a refinery, with no purchased feedstocks -- in particular, no alcohols.

- DIPE production could increase the refinery's overall conversion of FCC by-product streams into oxygenates and/or alkylates.

  A typical FCC unit produces more propylene (DIPE feedstock) than iso-butene (MTBE and ETBE feedstock) or iso-amylene (TAME and TAEE feedstock). Consequently, a typical FCC unit can support more captive oxygenate production with DIPE than with MTBE, ETBE, TAME, or TAEE. This phenomenon allows routing additional butenes and amylenes to alkylation to replace propylene or to support additional alkylate production. For various technical reasons (beyond the scope of this report), butenes and amylenes are more desirable than propylene as alkylation feed.

- DIPE is a higher-quality gasoline blendstock (with respect to both engine performance and vehicle emissions) than the other gasoline blendstocks derived from propylene (as Table 1 indicates).

  DIPE has a much higher octane than either propylene alkylate or polymer gasoline. DIPE has zero olefin content; polymer gasoline is 100% olefin. Under EPA's Complex Model for certifying federal RFG, reducing olefin content is a preferred means of reducing VOC and NOx emissions.

On the other hand, to the extent that DIPE capacity substitutes for captive MTBE capacity, refiners lose opportunities to exploit the price differential between methanol and ethanol. A captive ether (MTBE/ETBE) plant enables a refiner to use the cheaper alcohol and produce either MTBE or ETBE. A DIPE plant offers no comparable flexibility.

*Costs of DIPE Production*

In our prior work, the ARMS model included a representation of the DIPE process and the ARMS database included per-barrel cost factors -- capital investment, capital recovery rate, and operating cost elements -- for a grass roots DIPE unit. We derived the cost factors in the ARMS database from basic cost elements reported by UOP Inc. [UOP94] (**Table 2**).

The indicated capital investment for DIPE production is roughly comparable to that for captive MTBE production. In particular, the capital investment (per barrel of DIPE production capacity) quoted by UOP is about 125% that for a grass roots, captive MTBE unit (per barrel of MTBE production capacity).

The operating cost associated with DIPE production is lower than that for captive MTBE production, primarily because DIPE production requires no purchased alcohol.

**Table 2: Cost Factors for DIPE Production**

| | |
|---|---|
| Capital Investment (per Bbl/day of capacity)* | $5.6 M |
| Operating Cost Factors (per Bbl of DIPE) | |
| -- Power | 5.6 kW |
| -- Steam | 460 lb |
| -- Cooling Water | 900 gal |
| -- Catalyst Make-up | $1.0 |

* Inside battery limits (ISBL) investment, in 1994 dollars, for a grass roots plant producing 2,300 Bbl DIPE per stream day, at a U.S. Gulf Coast location

## Likely Evolution of DIPE Investment Costs Over Time

As discussed in the next section, our sensitivity analysis is "symmetical" with respect to DIPE investment costs: we consider the same range of investment levels above and below the baseline. One should not infer from this symmetry that the high and low ranges of investment are equally likely outcomes in 2010. The more prudent assumption is that DIPE investment costs (in real dollars, per barrel of capacity) will decrease as time goes on.

At first, this view may appear to run counter to experience. It is widely accepted that pioneering projects embodying new technology tend to incur significant over-runs in investment costs. Notable examples of investment over-runs include breeder reactors, coal gasification plants, oil shale extraction plants, and the supersonic passenger plane.

But over-runs are not common in the refining sector, even with new processes such as DIPE. In the refining sector, pioneering projects tend to come in on or close to budget, and investment (in real dollars, per unit of capacity) tends to decrease as subsequent units are built.

This experience is the result of a number of factors, such as:

- Over-design of pioneering units: Process licensors and engineering firms over-design projects that pioneer a new process technology. As they gather experience with the technology, they tighten their designs by reducing safety margins, cutting back on redundant equipment, and eliminating "gold plating".

- Evolutionary improvement in technology: As time goes on, technology improves -- both in general (e.g., materials of construction, process control) and with respect to a specific process (e.g., new process chemistry, improved catalysts, new process designs). For example, in TAME production, a new processing scheme -- catalytic distillation -- led to significant reductions in investment requirements and corresponding improvements in TAME economics.

- Competition: As a new refining process gains acceptance, the number of process licensors and engineering firms offering proprietary variants of the process tends to increase. The resulting competition drive downs vendors' bids on new process units and thereby reduces the investment costs incurred by refiners.

The DIPE process now offered by UOP, Inc. is new, and the pioneering commercial-scale unit is yet to be built. But DIPE production is an evolutionary, not a revolutionary, advance in refining process technology. DIPE chemistry is well understood, and the process design employs conventional equipment and operating conditions. DIPE investment requirements are likely to evolve as is customary in the refining sector -- that is, to decrease over time once the process has entered commercial use.

## Methodology for The Analysis

As in the prior work, we employed our generalized refinery modeling system, **ARMS**, in this study. In particular, we used ARMS to explore a series of cases representing a range of (1) investment requirements for DIPE process units, (2) demand for refinery propylene in the petrochemical sector, and (3) ethanol consumption in the refining sector.

Our analysis comprised three steps.

1. Set baseline refining capacity. Establish baseline refining capacity for 2010 by means of the ARMS model configuration and modeling database developed in the prior study for the scenario in which

   -- The crude oil price is at the **mid-range** level;

   -- The 1 psi RVP waiver is not in effect; and

   -- Refining capacity is optimized for production of

   - 50% RFG, without using ethanol either as a feedstock for ether production or as a direct gasoline blendstock, and
   - 50% conventional gasoline, using **100,000 Bbl/day** of ethanol as direct blendstock.

2. Develop refining capacity profiles as a function of DIPE economics. Starting with the baseline refining capacity profile derived in the first step, use ARMS to develop a set of new baseline refining capacity profiles for 2010. Each member of the set corresponds to a particular combination of (1) investment cost per unit of DIPE capacity and (2) level of petrochemical demand for propylene.

The eleven combinations considered are listed in **Table 3**. In Table 3, the percentages denote values relative to the corresponding values in the prior work (and in the baseline capacity profile for this analysis). Thus, 100% denotes a value equal to that used in the prior work; 150% denotes a value 50% higher than that used in the prior work; etc. The baseline (100%) value for capital investment is that shown in Table 2..

**Table 3: DIPE Investment and Propylene Demand Levels Treated in the Analysis**

| DIPE Investment [1] | Propylene Demand [2] |
|---|---|
| 100% | 100% |
| 125% | |
| 150% | |
| 75% | |
| 50% | |
| 100% | 125% |
| 125% | |
| 75% | |
| 100% | 150% |
| 125% | |
| 75% | |

Notes:
1. For **DIPE Investment**, 100% = $5.6 M per Bbl/day of capacity
2. For **Propylene Demand**, 100% = 130 M Bbl/day

3. Estimate the refining value of ethanol as a function of DIPE economics. From the eleven baseline refining capacity profiles derived in the preceding step, establish upper and lower bounds for potential DIPE production capacity in 2010. Then, use ARMS to generate the ethanol demand function for each of three levels of DIPE capacity:

   - High: 350 M Bbl/day
   - Mid-range: 220 (the baseline value, drawn from the prior study)
   - Low: 0

   We also considered a variant of the low (zero) DIPE production scenario, involving a high volume of MTBE imports (the oxygen equivalent of the mid-range DIPE volume).

   Generating ethanol demand functions for each level of DIPE capacity entails making a series of ARMS runs, with each run in a series corresponding to a different level of ethanol consumption in the refining sector. In each run, ARMS returns a refining value for the specified level of ethanol consumption (and the specified DIPE production capacity).

**Results of the Analysis**

As noted above, this analysis embodies assumptions that (1) the world oil price follows the mid-range trajectory out to 2010 and (2) RFG constitutes 50% of the U.S. gasoline pool in 2010. Given these assumptions, the primary results and findings of this analysis are as follows.

*Projected DIPE Capacity*

- The projected volume of on-stream DIPE capacity in 2010 is a strong inverse function of the investment cost per unit of of DIPE capacity.

  As **Chart 1** (at the back of this report) illustrates, indicated DIPE production capacity in 2010 decreases monotonically from 545 M Bbl/day to zero as the DIPE investment cost increases from 50% to 150% of the baseline value (Table 2). Consistent with the results of the prior work, indicated DIPE production capacity is 220 M Bbl/day at the baseline DIPE investment (and the baseline propylene demand).

- The projected amount of on-stream DIPE capacity in 2010 is independent of the demand for refinery propylene in the petrochemical sector.

  As **Chart 2** illustrates, indicated DIPE production capacity in 2010 is insensitive to increases in the petrochemical sector's demand for refinery propylene, up to at least 150% of baseline demand.

  As noted earlier, U.S. refineries can increase propylene production through suitable adjustment of FCC operating conditions and selection of FCC catalysts. In particular, they can increase propylene production enough to meet even the largest projected increase in propylene demand, with minor increases in refining costs.

- DIPE production capacity in 2010 is likely to range from 150 to 350 M Bbl/day, depending on the investment cost for DIPE capacity.

  These bounds correspond to 125% and 75%, respectively, of the baseline capital investment per unit of DIPE capacity. (As discussed earlier, the lower value for capital investment should be considered more likely in 2010 than the higher value.)

*Effects of DIPE Capacity on Ethanol's Refining Value*

For brevity, let **EV** = ethanol volume consumed in the U.S. refining sector (in M Bbl/day). Then, our results may be expressed as follows.

- For **EV $\leq$ 400**, ethanol's refining value is independent of DIPE volume (and, by implication, of DIPE economics).

- For **400 < EV $\leq$ 500**, ethanol's refining value is a weak decreasing function of DIPE capacity. In particular, at **EV = 500**, ethanol's refining value decreases by about 3 ¢/gal as DIPE capacity increases over the full range considered (0 ---> 350 M Bbl/day).

- For **EV > 500**, ethanol's refining value is a strong decreasing function of DIPE capacity. Similarly, the maximum ethanol volume that can yield a refining value of at least $27/Bbl (65 ¢/gal) is a strong decreasing function of DIPE capacity. It decreases from 600 M Bbl/day to 500 M Bbl/day as DIPE capacity increases over the full range considered (0 ---> 350 M Bbl/day).

  **Chart 3** illustrates these results, in terms of the ethanol demand functions estimated for the four DIPE capacity scenarios considered: (1) high (350 M Bbl/day), (2) mid-range (220 M Bbl/day), (3) zero capacity (with baseline MTBE imports), and (4) zero capacity (with high MTBE imports). (The fourth scenario embodies an increase in the volume of MTBE imports equivalent (in terms of oxygen content) to 220 M Bbl/day of DIPE.)

These results reflect the following factors.

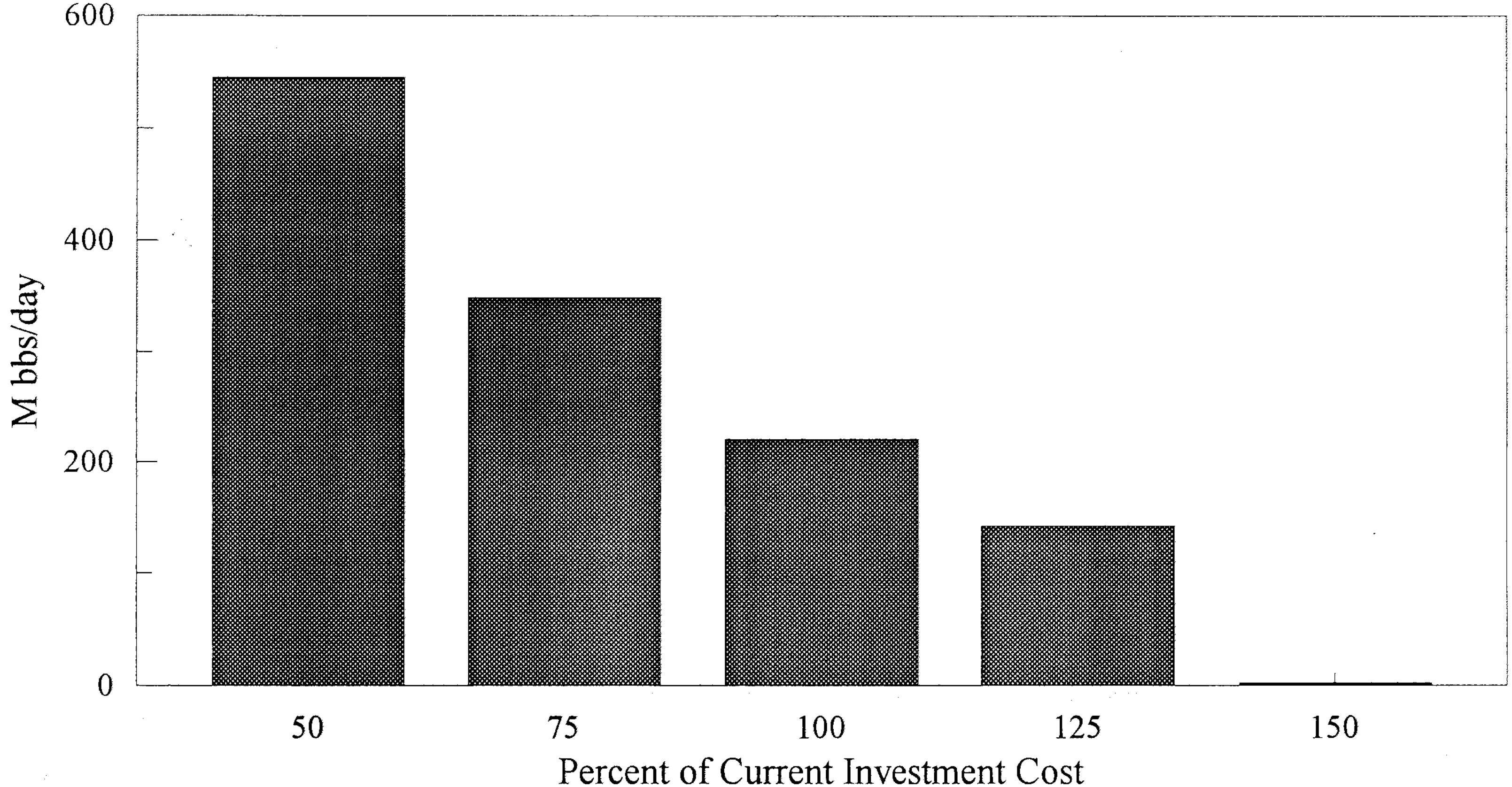
As in the prior study, this analysis allocates the first 400 M Bbl/day of refinery ethanol consumption to conventional gasoline, and all additional ethanol consumption to RFG (as ether feedstock). DIPE capacity displaces merchant supplies of MTBE and future additions to captive ether capacity -- MTBE or ETBE, depending on the relative prices of methanol and ethanol. The displacement of ether capacity by DIPE capacity reduces the volume of ethanol that the refining sector can absorb (except at ethanol prices too low to be interesting). For any given level of MTBE imports, there is a corresponding volume of captive ether plant capacity, dictated by the oxygen requirement of the RFG pool. Increasing MTBE imports progressively diminishes the potential volume of this outlet for ethanol.

**References**

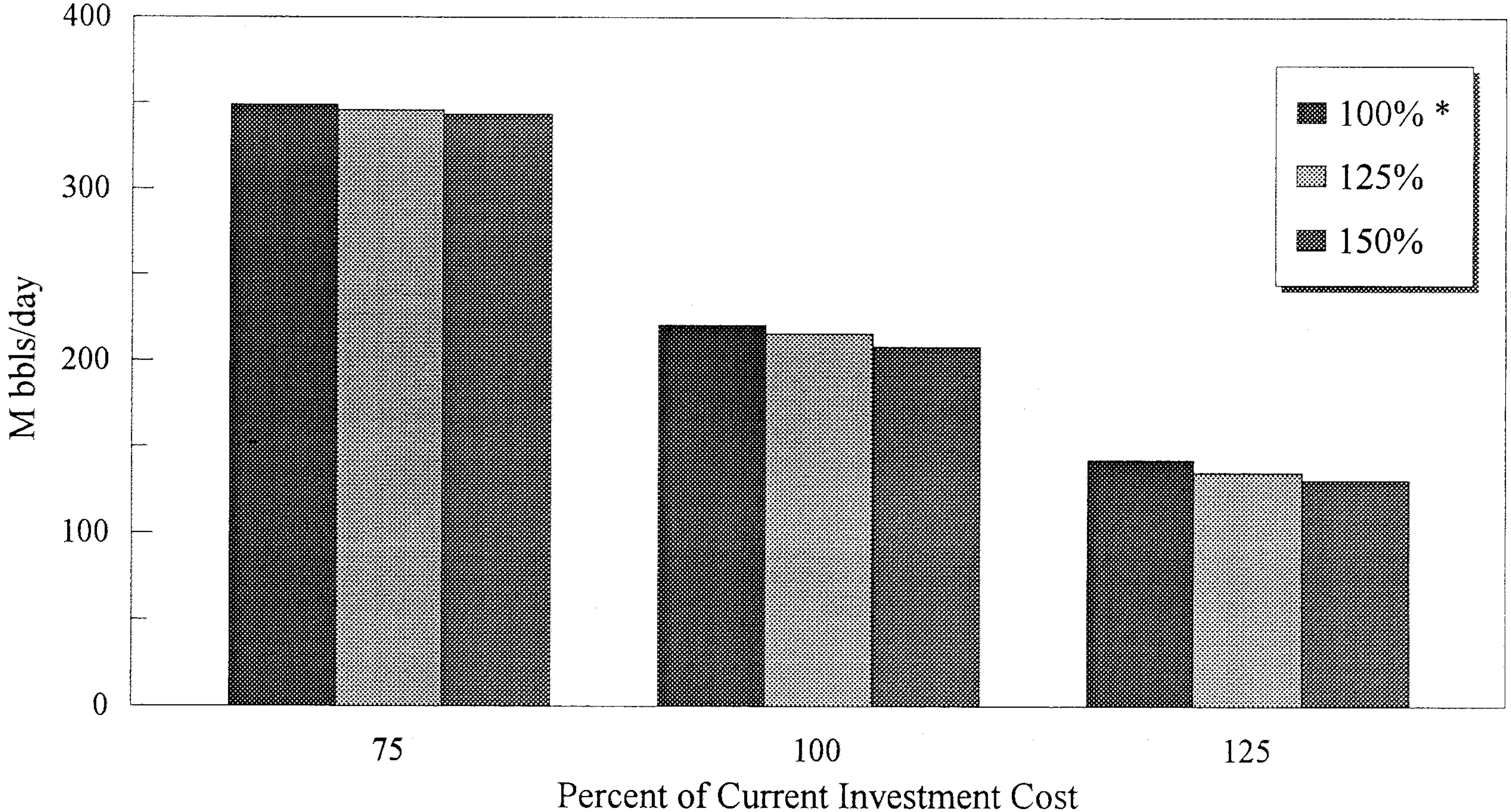
[MP95]: *The Refining Value of Ethanol as Gasoline Blendstock and Ether Feedstock*, prepared by MathPro Inc. under subcontract to Information Resources, Inc. for NREL, under Contract No. AAW-4-14215-01, 18 July 1995

[UOP94]: *Low-Cost DIPE Production*, Marker, T. L., et al, Proceedings of the 1994 Conference on Clean Air Act and Reformulated Gasolines, Information Resources, Inc., 9-11 October 1994

Chart 1: Projected DIPE Capacity, by Investment Cost Scenario



## Chart 2: Projected DIPE Capacity, by Investment Cost and Propylene Sales Scenarios




* Percent of Projected Propylene Sales for 2010

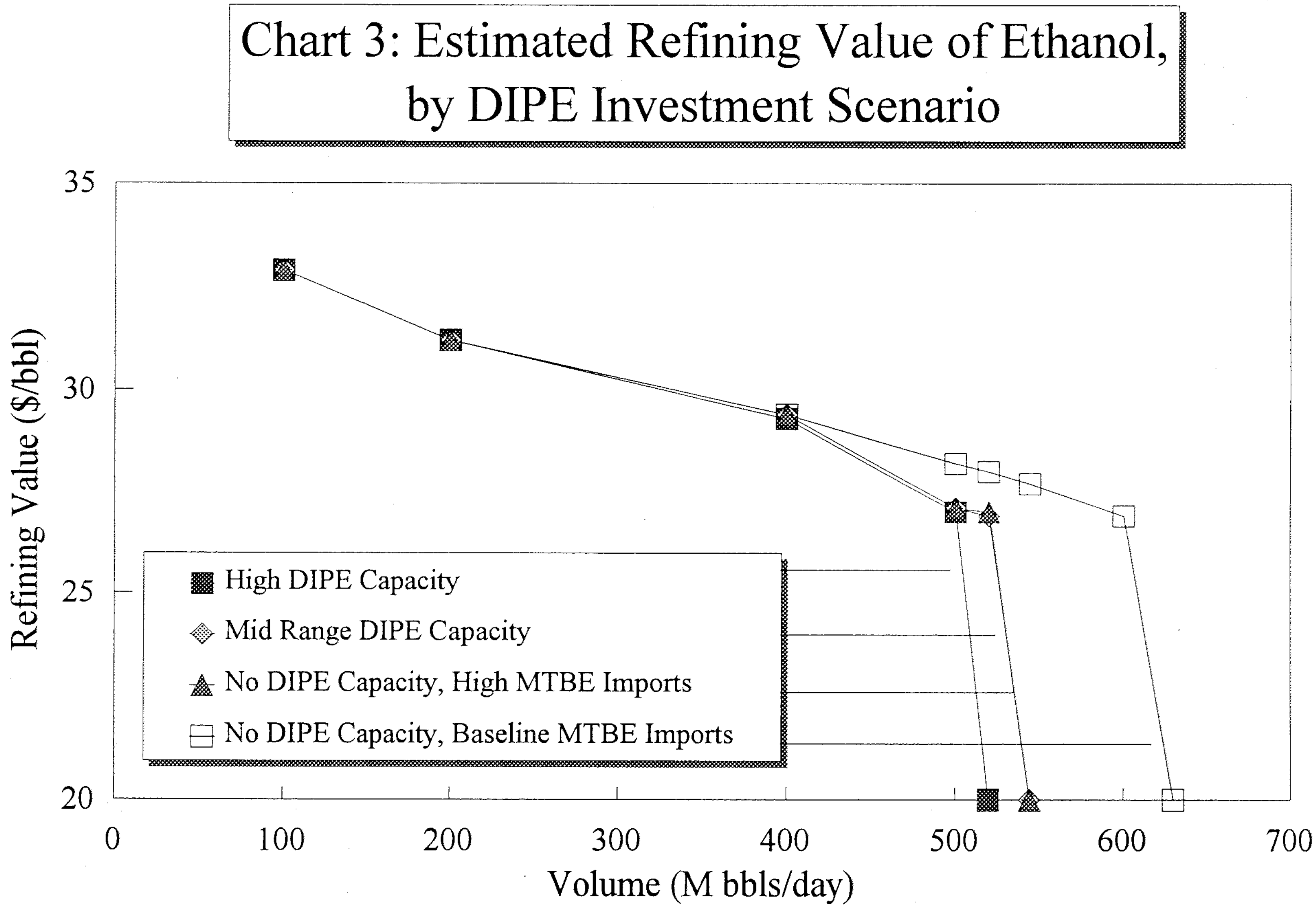


Chart 3: Estimated Refining Value of Ethanol, by DIPE Investment Scenario
35
30
25
20
Refining Value ($/bbl)
0
100
200
300
400
500
600
700
Volume (M bbls/day)
High DIPE Capacity
Mid Range DIPE Capacity
No DIPE Capacity, High MTBE Imports
No DIPE Capacity, Baseline MTBE Imports

# Table 1: Estimated Refining Value of Ethanol, by DIPE Investment Cost Scenario

### (for Mid Range Oil Price Scenario)

| DIPE Investment Cost Scenario | Ethanol Volume (M bbls/d) | | | Refining Value/Cost | |
|---|---|---|---|---|---|
| | Conventional Gasoline | Ether Feed | Total | Ethanol ($/bbl) | Conventional Gasoline ($/bbl) |
| 75% of Current | 100 | | 100 | 32.90 | 33.00 |
| | 200 | | 200 | 31.20 | 28.00 |
| | 400 | | 400 | 29.30 | 27.00 |
| | 400 | 100 | 500 | 27.00 | 27.00 |
| | 400 | 120 | 520 | 20.00 | 27.00 |
| Current | 100 | | 100 | 32.90 | 33.00 |
| | 200 | | 200 | 31.20 | 29.00 |
| | 400 | | 400 | 29.40 | 27.00 |
| | 400 | 120 | 520 | 26.90 | 27.00 |
| | 400 | 145 | 545 | 22.10 | 27.00 |
| 150% of Current (high MTBE Imports) | 100 | | 100 | 32.90 | 33.00 |
| | 200 | | 200 | 31.20 | 29.00 |
| | 400 | | 400 | 29.40 | 27.00 |
| | 400 | 100 | 500 | 27.10 | 27.00 |
| | 400 | 120 | 520 | 27.00 | 27.00 |
| | 400 | 145 | 545 | 20.00 | 27.00 |

# Table 2: Oxygenate Volumes, byType and DIPE Investment Cost Scenario

**(for Mid Range Oil Price Scenario)**

**(M bbls/day)**

| DIPE Investment Cost Scenario* | Total Ethanol | Type of Oxygenate | | | | | | |
|---|---|---|---|---|---|---|---|---|
| | | MTBE | | | | | | |
| | | Captive | Merchant | ETBE | TAME | TAEE | DIPE | Ethanol |
| 75% of Current | 102 | 163 | 80 | 2 | 12 | 0 | 297 | 101 |
| | 202 | 160 | 41 | 2 | 0 | 0 | 296 | 201 |
| | 401 | 160 | 40 | 1 | 1 | 2 | 296 | 400 |
| | 500 | 0 | 12 | 221 | 0 | 0 | 296 | 400 |
| | 520 | 0 | 0 | 265 | 0 | 1 | 296 | 400 |
| Current | 102 | 154 | 130 | 2 | 12 | 0 | 188 | 101 |
| | 202 | 157 | 80 | 0 | 10 | 3 | 245 | 201 |
| | 401 | 156 | 80 | 0 | 9 | 3 | 247 | 400 |
| | 520 | 0 | 11 | 258 | 4 | 9 | 249 | 400 |
| | 545 | 0 | 0 | 313 | 4 | 9 | 207 | 400 |
| 150% of Current (with high MTBE Imports) | 102 | 227 | 130 | 2 | 116 | 0 | 0 | 101 |
| | 202 | 277 | 80 | 2 | 116 | 0 | 0 | 201 |
| | 401 | 279 | 80 | 0 | 113 | 3 | 0 | 400 |
| | 520 | 116 | 80 | 191 | 38 | 87 | 0 | 400 |
| | 600 | 0 | 44 | 368 | 38 | 87 | 0 | 400 |
| | 630 | 0 | 0 | 418 | 21 | 105 | 0 | 400 |

* Production of DIPE is 85% of nameplate capacity.